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Rational designing of phenothiazine dioxide based hole transporting materials for efficient perovskite solar cells

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Abstract

In this study, we design five novel non-fullerene end capped acceptor based efficient hole transporting materials (HTMs) from phenothiazine dioxide-based core. MPW1PW91 functional with a 6-31G basis set was employed for all DFT calculations and simulation analysis. By substituting acceptor groups in PDO2, numbers of parameters like band gaps, the frontier molecular orbitals (FMOs), higher absorption parameters, and electronic properties like ionization potential, electron affinity, binding energy, and light harvesting efficiency (LHE) were well tuned. In addition, significant variations in other geometrical parameters such as dipole moment, and reorganizational energy parameters were also noticed for the derived molecules compared to the reference molecule (R). Device performance was analyzed by performing calculations of open circuit voltage (V_{OC}) and fill factor (FF). Consequently, all the designed derivatives demonstrated an improved V_{OC} of 0.84V for an optimized designed structure. In comparison, it was limited to a V_{OC} of 0.57V for the reference (R) PDO2, displaying an increment in efficiency which is essential to use these molecules as highly efficient HTMs for perovskite solar cell devices in the future.